(FILE 'CAPLUS' ENTERED AT 08:56:50 ON 24 MAR 2004)
DEL HIS

L1	1860216	S	PROTEIN
L2	237352	S	CRYSTALLIZATION
L3	1691	S	COCRYSTALLIZATION
L4	238015	S	L2 OR L3
L5	5438	S	L1 (L) L4
L6	230781	S	SINGLE CRYSTAL
L7	314375	S	LATTICE
L8	444901	S	MATRIX
L9	570	S	L5 AND (L6 OR L7 OR L8)
L10	436856	S	CRYSTAL STRUCTURE
L11	215	S	L9 AND L10
L12	134105	S	INCLUSION
L13	17966	S	ENTRAP?
L14	151082	S	L12 OR L13
L15	1	S	L11 AND L14
L16	215	S	L11
L17	1	S	2000:900424/AN
L18	1	S	1999:422851/AN
L19	95	S	L1 AND L3
L20	17	S	L19 AND (L6 OR L7 OR L8 OR L12 OR L13)
L21	129112	S	STABILIZATION
L22	2583	S	L1 AND L4 AND L10
L23	166	S	L22 AND L6
L24	165	S	L23 NOT L20
L25	7	S	L24 AND (L7 OR L8)

L20 ANSWER 1 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:101291 CAPLUS
DOCUMENT NUMBER: 140:177313
TITLE: Cloning and physical characterization of deoxyuridine 5'-triphosphatase from pathogenic bacteria and their use as antimicrobial targets
INVENTOR(S): Edwards, Aled; Dharamsi, Akil; Vedadi, Masoud; Domagala, Megan; Mansoury, Kamran; Kimber, Matthew; Houston, Simon; Awrey, Donald; Beattie, Bryan
PATENT ASSIGNEE(S): Affinium Pharmaceuticals, Inc., Can.
SOURCE: PCT Int. Appl., 220 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004011638	A2	20040205	WO 2003-CA1129	20030731
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
WO 2003087354	A2	20031023	WO 2003-CA485	20030408
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.:

US 2002-399971P	P	20020731
WO 2003-CA485	A	20030408
US 2002-371067P	P	20020409
US 2002-386548P	P	20020605
US 2002-386826P	P	20020606
US 2002-386869P	P	20020606
US 2002-424380P	P	20021106
US 2002-425086P	P	20021108
US 2002-436243P	P	20021224
US 2002-436288P	P	20021224
US 2002-436566P	P	20021226
US 2002-436567P	P	20021226
US 2002-436708P	P	20021227
US 2002-436947P	P	20021230
US 2002-436971P	P	20021230
US 2002-437038P	P	20021230
US 2002-437141P	P	20021230
US 2002-437620P	P	20021231
US 2002-437638P	P	20021231

AB The present invention relates to novel drug targets for pathogenic bacteria. Reliable, high throughput methods are developed to identify, express, and purify deoxyuridine 5'-triphosphatase from Enterococcus faecalis and Streptococcus pneumoniae. The nucleic acid and encoded amino acid sequences for the deoxyuridine 5'-triphosphatase from E. faecalis and S. pneumoniae are provided. The invention also provides bioinformatic, biochem. and biophys. characteristics of the polypeptides of the invention, in particular characterization by mass spectrometry, NMR spectrometry, and x-ray crystallog. Crystal structure of deoxyuridine 5'-triphosphatase from S. pneumoniae is provided.

L20 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:855956 CAPLUS
DOCUMENT NUMBER: 139:347484
TITLE: Cloning, sequence, crystal structure and physical

characterization of (3R)-hydroxymyristoyl-(acyl-carrier-**protein**) dehydratase from Pseudomonas aeruginosa and its use as antimicrobial target

INVENTOR(S): Edwards, Aled; Dharamsi, Akil; Vedadi, Masoud; Domagala, Megan; McDonald, Merry-Lynn; Houston, Simon; Vallee, Francois; Kimber, Matthew; Awrey, Donald; Beattie, Bryan

PATENT ASSIGNEE(S): Affinium Pharmaceuticals, Inc., Can.

SOURCE: PCT Int. Appl., 304 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003089463	A1	20031030	WO 2003-CA560	20030417

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2002-373321P P 20020417

AB The present invention relates to novel drug targets for pathogenic bacteria. Reliable, high throughput methods are developed to identify, express, and purify (3R)-hydroxymyristoyl-(acyl-carrier-**protein**) dehydratase from P. aeruginosa. The invention provides the nucleic acid sequence and the encoded amino acid sequence of the enzyme. The invention also provides crystal structure and other biochem. and biophys. characteristics of the P. aeruginosa (3R)-hydroxymyristoyl-(acyl-carrier-**protein**) dehydratase.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:595584 CAPLUS

DOCUMENT NUMBER: 137:274987

TITLE: Substrate Binding Induces a Cooperative Conformational Change in the 12S Subunit of Transcarboxylase: Raman Crystallographic Evidence

AUTHOR(S): Zheng, Xiaojing; Rivera-Hainaj, Rosa E.; Zheng, Yuangang; Pusztai-Carey, Marianne; Hall, Pamela R.; Yee, Vivien C.; Carey, Paul R.

CORPORATE SOURCE: Department of Biochemistry and Department of Pharmacology, Case Western Reserve University, Cleveland, OH, 44106, USA

SOURCE: Biochemistry (2002), 41(35), 10741-10746
CODEN: BICHAW; ISSN: 0006-2960

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The 12S subunit of transcarboxylase is a 338,000 Da hexamer that transfers carboxylate from methylmalonyl-CoA (MM-CoA) to biotin; in turn, the biotin transfers the carboxylate to pyruvate on another subunit, the 5S. Here, Raman difference microscopy is used to study the binding of substrate and product, and their analogs, to **single crystals** of 12S. A **single crystal** is the medium of choice because it provides Raman data of unprecedented quality. Crystalline ligand-**protein** complexes were formed by **cocrystn.** or by the soaking in/soaking out method. Raman difference spectra were obtained by subtracting the spectrum of the apo crystal from that of a crystal with the substrate or product bound. Raman difference spectra from crystals with the substrate bound are dominated by bands from the **protein** 's amide bonds and aromatic side chain residues. In contrast, Raman difference spectra involving the product, propionyl-CoA, are dominated by modes from the ligand. These results show that substrate binding triggers a conformational change in 12S, whereas product binding does not. The conformational change involves an increase in the amount of α-helix since markers for this secondary structure are prominent in the difference spectra of the substrate complex. The number of MM-CoA ligands bound per 12S

hexamer can be gauged from the intensity of the MM-CoA Raman features and the fact that the **protein** concentration in the crystals is known from x-ray crystallog. data. Most crystal samples had six MM-CoAs per hexamer although a few, from different soaking expts., contained only 1-2. However, both sets of crystals showed the same degree of **protein** conformational change, indicating that the change induced by the substrate is cooperative. This effect allowed us to record the Raman spectrum of bound MM-CoA without interference from **protein** modes; the Raman spectrum of a 12S crystal containing 2 MM-CoA ligands per hexamer was subtracted from the Raman spectrum of a 12S crystal containing six MM-CoA ligands per hexamer. The conformational change is reversible and can be controlled by soaking out or soaking in the ligand, using either concentrated ammonium sulfate solns. or the solution used in the crystallization trials. Malonyl-CoA also binds to 12S crystals and brings about conformational changes identical to those seen for MM-CoA; in addition, butyryl-CoA binds and behaves in a manner similar to propionyl-CoA. These data implicate the -COO- group on MM-CoA (that is transferred to biotin in the reaction on the intact enzyme) as the agent bringing about the cooperative conformational change in 12S.

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:564616 CAPLUS
DOCUMENT NUMBER: 138:309053
TITLE: Hybrid insulin cocrystals for controlled release delivery
AUTHOR(S): Brader, Mark L.; Sukumar, Muppalla; Pekar, Allen H.; McClellan, David S.; Chance, Ronald E.; Flora, David B.; Cox, Amy L.; Irwin, Lynnie; Myers, Sharon R.
CORPORATE SOURCE: Lilly Research Laboratories, Bioproduct Pharmaceutical Development, Eli Lilly and Company, Indianapolis, IN, 46285, USA
SOURCE: Nature Biotechnology (2002), 20(8), 800-804
CODEN: NABIF9; ISSN: 1087-0156
PUBLISHER: Nature Publishing Group
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The ability to tailor the release profile of a drug by manipulating its formulation **matrix** offers important therapeutic advantages. We show here that human insulin can be cocrystd. at preselected ratios with the fully active lipophilically modified insulin derivative octanoyl-Nε-LysB29-human insulin (C8-HI). The cocrystal is analogous to the NPH (neutral protamine Hagedorn) crystalline complex formed with human insulin, which is commonly used as the long-acting insulin component of diabetes therapy. The in vitro and in vivo release rates of the cocrystal can be controlled by adjusting the relative proportions of the two insulin components. We identified a cocrystal composition comprising 75% C8-HI and 25% human insulin that exhibits near-ideal basal pharmacodynamics in somatostatin-treated beagle dogs. The dependence of release rate on cocrystal ratio provides a robust mechanism for modulating insulin pharmacodynamics. These findings show that a crystalline **protein matrix** may accommodate a chemical modification that alters the dissoln. rate of the crystal in a therapeutically useful way, yet that is structurally innocuous enough to preserve the pharmaceutical integrity of the original microcryst. entity and the pharmacol. activity of the parent mol.

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:869148 CAPLUS
DOCUMENT NUMBER: 136:50548
TITLE: Manipulation of temperature to improve solubility of hydrophobic **proteins** and **cocrystallization** with **matrix** for analysis by MALDI-TOF mass spectrometry
AUTHOR(S): Bird, Gregory H.; Lajmi, Ajay R.; Shin, Jumi A.
CORPORATE SOURCE: Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE: Analytical Chemistry (2002), 74(1), 219-225
CODEN: ANCHAM; ISSN: 0003-2700
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB **Matrix**-assisted laser desorption/ionization mass spectrometry (MALDI-MS) requires **cocrystn.** of analyte with a large excess of **matrix**, which must be mutually soluble in a solvent that encourages

crystal growth upon evaporation MALDI-MS of hydrophobic **proteins** can be difficult, because they tend to aggregate in polar solns. High concns. of denaturants and salts are often employed to combat **protein** aggregation, but this can result in signal suppression. By using various organic cosolvent systems and **matrixes** at different **protein** :**matrix** ratios, we were able to use MALDI-TOFMS to detect four bacterially expressed hydrophobic **proteins** comprising alanine-rich mutants of the basic region/leucine zipper **protein** (bZIP) GCN4. By manipulating sample temperature, we were able to maintain **protein** solubility **Protein** aggregation was suppressed when mixing the **protein** and **matrix** solns. at 4° prior to warming to 37°, following the temperature-leap technique described by Xie and Wetlaufer (**Protein** Sci. 1996, 5, 517-523), who used this method to renature bovine carbonic anhydrase II. Manipulation of temperature encouraged our hydrophobic **proteins** to adopt conformations leading to the nonaggregating state, and solubility was maintained even when the concentration of denaturant was reduced from 4 M to 400 mM. The temperature-leap tactic was critical for maintaining **protein** solubility, preventing signal suppression normally seen with higher concns. of salts, allowing for generation of superior spectra, and should prove applicable to other systems prone to aggregation.

REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:612367 CAPLUS
DOCUMENT NUMBER: 136:49854
TITLE: Crystallization of bFGF-DNA aptamer complexes using a Sparse **Matrix** designed for **protein** -nucleic acid complexes
AUTHOR(S): Cannone, J. J.; Barnes, C. L.; Achari, A.; Kundrot, C. E.
CORPORATE SOURCE: University of Texas at Austin, Institute for Cellular and Molecular Biology, Austin, TX, 78712-1095, USA
SOURCE: Journal of Crystal Growth (2001), 232(1-4), 409-417
CODEN: JCRGAE; ISSN: 0022-0248
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The Sparse **Matrix** approach for obtaining lead crystallization conditions has proven to be very fruitful for the crystallization of **proteins** and nucleic acids. Here we report a Sparse **Matrix** developed specifically for the crystallization of **protein**-DNA complexes. This method is rapid and economical, typically requiring 2.5 mg of complex to test 48 conditions. The method was originally developed to crystallize basic fibroblast growth factor (bFGF) complexed with DNA sequences identified through in vitro selection, or SELEX, methods. Two DNA aptamers that bind with approx. nanomolar affinity and inhibit the angiogenic properties of bFGF were selected for co-crystallization The Sparse **Matrix** produced lead crystallization conditions for both bFGF-DNA complexes.

REFERENCE COUNT: 93 THERE ARE 93 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:284412 CAPLUS
DOCUMENT NUMBER: 134:337776
TITLE: Mass spectrometric imaging of immobilized pH gradient gels and creation of "virtual" two-dimensional gels
AUTHOR(S): Walker, Angela K.; Rymar, Gary; Andrews, Philip C.
CORPORATE SOURCE: Department of Biological Chemistry, University of Michigan, Ann Arbor, MI, 48109-0606, USA
SOURCE: Electrophoresis (2001), 22(5), 933-945
CODEN: ELCTDN; ISSN: 0173-0835
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We have developed a **matrix** assisted laser desorption/ionization-time of flight (MALDI-TOF) based technique for the detection of intact **proteins** directly from immobilized pH gradient gels (IPGs). The use of this technique to visualize **proteins** from IPGs was explored in this study. Whole cell Escherichia coli exts. of various loadings were separated on IPGs. These IPGs were processed to remove contaminants and to achieve **matrix**/analyte **cocrystn.** on the surface of the gel. Mass spectra were acquired by scanning the surface of the gel and were assimilated into a "virtual" two dimensional (2-D) gel. This virtual 2-D gel is analogous to a "classical" 2-D gel, except that the mol. weight information is acquired by mass spectrometry

rather than by SDS-PAGE (SDS-PAGE). This mass spectrometry (MS) based technol. exemplifies a number of desirable characteristics, some of which are not attainable with classical two-dimensional electrophoresis (2-DE). These include high sensitivity, high reproducibility, and an inherently higher resolution and mass accuracy than 2-D gels. Furthermore, there is a difference in selectivity exhibited between virtual 2-D gels and classical 2-D gels, as a number of **proteins** are visible in the virtual gel image that are not present in the stained gels and vice versa. In this report, virtual 2-D gels will be compared to classical 2-D gels to illustrate these features.

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:333410 CAPLUS
TITLE: Chiral domain formation in **cocrystallization** of wild-type and mutant streptavidin.
AUTHOR(S): Farah, Sammy J.; Wang, Szu-Wen; Robertson, Channing R.; Gast, Alice P.
CORPORATE SOURCE: Department of Chemical Engineering, Stanford University, Stanford, CA, 94305-5025, USA
SOURCE: Book of Abstracts, 219th ACS National Meeting, San Francisco, CA, March 26-30, 2000 (2000), PHYS-292. American Chemical Society: Washington, D. C. CODEN: 69CLAC
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English
AB We are studying the macroscopic morphol. and mol. arrangement of two-dimensional streptavidin crystals bound to biotinylated lipid monolayers at the air-water interface. At pH 4, wild type streptavidin forms thin needle-like crystal structures with P1 **lattice** spacing. Using mol. modeling we identified the **protein-protein** contacts characteristic to this **lattice** structure. One of these contact points, an aspartate residue at position 36, was mutated to a lysine residue through recombinant **protein** techniques. The lysine residue was introduced to create steric and electrostatic repulsion at this contact point so as to disrupt formation of the P1 crystals. Unlike the wild type streptavidin at pH 4, the mutant streptavidin forms dendritic x-shaped crystals with P2 **lattice** spacing. Co-crystallization of wild type and mutant streptavidin was performed in varying ratios of each **protein** type. When 25% mutant streptavidin is introduced into the system, the needle-like crystals normally formed by wild type streptavidin begin to form with chiral ends. At 50% mutant concentration, the streptavidin crystals emerge with inverse-S shaped chiral morphologies. And when the mutant streptavidin concentration is increased to 75%, the crystals maintain their chirality, but become thinner. We believe that the chirality observed in these intermediate crystals is due to a combination of P1 and P2 **lattice** spacing within each crystal domain. These crystals are analogous in shape and structure to those formed from wild type streptavidin at lipid monolayers over a subphase pH range of 5 to 6. Here the electrostatic interactions cause a mixture of crystal types near the isoelec. point. We discuss these analogous systems and the nature of the solid-solid phase transition.

L20 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:453207 CAPLUS
DOCUMENT NUMBER: 131:210498
TITLE: DNA protection by stress-induced biocrystallization
AUTHOR(S): Wolf, Sharon G.; Frenkiel, Daphna; Arad, Talmon; Finkel, Steven E.; Kolter, Roberto; Minsky, Abraham
CORPORATE SOURCE: Departments of Organic Chemistry and Structural Biology, The Weizmnannl Institute of Science, Rehovot, 76100, Israel
SOURCE: Nature (London) (1999), 400(6739), 83-85 CODEN: NATUAS; ISSN: 0028-0836
PUBLISHER: Macmillan Magazines
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The crystalline state is considered to be incompatible with life. However, in living systems exposed to severe environmental assaults, the sequestration of vital macromols. in intracellular crystalline assemblies may provide an efficient means for protection. Here we report a generic defense strategy found in Escherichia coli, involving co-crystallization of its DNA with the stress-induced **protein** Dps. We show that when purified Dps and DNA interact, extremely stable crystals form almost instantaneously, within which DNA is sequestered and effectively protected against varied assaults. Crystalline structures with similar **lattice** spacings are formed in E. coli in which Dps is slightly over expressed, as well as in

starved wild-type bacteria. Hence, DNA-Dps co-crystallization is proposed to represent a binding mode that provides wide-range protection of DNA by sequestration. The rapid induction and large-scale production of Dps in response to stress, as well as the presence of Dps homologs in many distantly related bacteria, indicate that DNA protection by biocrystn. may be crucial and widespread in prokaryotes.

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:682554 CAPLUS
DOCUMENT NUMBER: 127:316127
TITLE: Access to phosphorylation in isocitrate dehydrogenase may occur by domain shifting
AUTHOR(S): Finer-Moore, Janet; Tsutakawa, Susan E.; Cherbavaz, Diana B.; LaPorte, David C.; Koshland, Daniel E., Jr.; Stroud, Robert M.
CORPORATE SOURCE: Department of Biochemistry and Biophysics, University of California, San Francisco, CA, 94143-0448, USA
SOURCE: Biochemistry (1997), 36(45), 13890-13896
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB To further clarify the mechanism of regulation by phosphorylation of Escherichia coli isocitrate dehydrogenase (I), **cocrystn.** of I and isocitrate dehydrogenase kinase/phosphatase (II) in the presence of an ATP analog was attempted. Although **cocrystn.** was unsuccessful, a new crystal form of I was obtained which provided insight into the phosphorylation mechanism. The new, orthorhombic crystal form of I was related to the previously reported tetragonal form largely by an .apprx.16° shift of a large domain relative to the small domain and clasp region within each subunit of the dimeric enzyme. The NADP cofactor binding surface was significantly disrupted by the shift to the open conformation. The solvent-accessible surface area and surface-enclosed volume increased by 2% relative to the dimeric tetragonal form. Most of the increase resulted from expansion of the active site cleft such that the distance across its opening increased from .apprx.5 to 13 Å, significantly increasing accessibility to Ser-113. The conformation of I in the orthorhombic crystal form more closely resembled that of the crystal structure of the homologous enzyme, 3-isopropylmalate dehydrogenase, than did the tetragonal I conformation. Since the crystal **lattice** forces are fairly weak, it appears that I is a flexible mol. that can easily undergo domain shifts and possibly other induced-fit conformational changes, to accommodate binding to II.

L20 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:230230 CAPLUS
TITLE: Precipitation-coprecipitation reactions mechanics in **protein** isolation.
AUTHOR(S): Lovrien, Rex; Matulis, Daumantas
CORPORATE SOURCE: Biochemistry Dept., Univ. Minnesota, St. Paul, MN, 55108, USA
SOURCE: Book of Abstracts, 213th ACS National Meeting, San Francisco, April 13-17 (1997), BIOC-164. American Chemical Society: Washington, D. C.
CODEN: 64AOAA
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English

AB Precipitative isolations of **proteins** till about 1950 were described as "methods": Salting out, etc. Older, and newer precipitative means can be understood now in two respects: (i) Mol. mechanics. (ii) Thermodn. outlines. The mechanics now focus on **protein** conformational motility, and **protein** hydration. Precipitative R and D needs start with these aspects to develop new means and get control of older methods. The thermodn. basis is either increase chemical potential of **proteins** in solution, decrease it for ppts., or both. Salting out is a hybrid of both. Realistic concepts of **protein** mol. mechanics enable design of a new precipitative methods, **matrix** ligand copptn.-**cocrystn.**, and entanglement ligand methods. It is practical now to selectively bring down **proteins** from 0.1% solns., with good protection of enzymes so precipitated This enables faster, more severe operating conditions to be used. **Matrix** and entanglement ligands enable one to control precipitate densities and graininess, to ease process steps.

L20 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1994:75673 CAPLUS

DOCUMENT NUMBER: 120:75673
TITLE: Encapsulation of food ingredients
AUTHOR(S): Shahidi, Fereidoon; Han, Xiao Qing
CORPORATE SOURCE: Dep. Biochem., Mem. Univ. Newfoundland, St. John's, NF, A1B 3X9, Can.
SOURCE: Critical Reviews in Food Science and Nutrition (1993), 33(6), 501-47
CODEN: CRFND6; ISSN: 1040-8398
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review with 239 refs. Microencapsulation is a relatively new technol. that is used for protection, stabilization, and slow release of food ingredients. The encapsulating or wall materials used generally consist of starch, starch derivs. **proteins**, gums, lipids, or any combination of them. Methods of encapsulation of food ingredients include spray-drying, freeze-drying, fluidized bed-coating, extrusion, **cocrystn.**, mol. **inclusion**, and coacervation. This paper reviews techniques for preparation of microencapsulated food ingredients and choices of coating material. Characterization of microcapsules, mechanisms of controlled release, and efficiency of protection/stabilization of encapsulated food ingredients are also presented.

L20 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:55470 CAPLUS
DOCUMENT NUMBER: 118:55470
TITLE: **Matrix** coprecipitating and cocrystallizing ligands (MCC ligands) for bioseparations
AUTHOR(S): Conroy, Mark J.; Lovrien, Rex E.
CORPORATE SOURCE: Biochem. Dep., Univ. Minnesota, St. Paul, MN, 55108, USA
SOURCE: Journal of Crystal Growth (1992), 122(1-4), 213-22
CODEN: JCRGAE; ISSN: 0022-0248
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Instead of trying to crystallize or precipitate amino acids and **proteins** as homogeneous products, often it is easier to coppt. or to cocrystallize them. Organic ionic ligands with large apolar groups bind to the solute or compound that is to be isolated. The resulting complexes come out of solution as coppts., often as cocrystals. Binding isotherms, Job plot anal., compositional and calorimetric data give combining stoichiometries for **matrix** ligands to amino acids, dipeptides, and **proteins**. These are 1:1 or 2:1, for amino acids and dipeptides, in cocryst. complexes. Coppts. of lysozyme and α-chymotrypsin bind anionic ligands strongly in combining ratios very close to **protein** net proton charge.

L20 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:404023 CAPLUS
DOCUMENT NUMBER: 115:4023
TITLE: The open/closed conformational equilibrium of aspartate aminotransferase. Studies in the crystalline state and with a fluorescent probe in solution
AUTHOR(S): Picot, Daniel; Sandmeier, Erika; Thaller, Christina; Vincent, Michael G.; Christen, Philipp; Jansonius, Johan N.
CORPORATE SOURCE: Abt. Strukturbiol., Univ. Basel, Basel, CH-4056, Switz.
SOURCE: European Journal of Biochemistry (1991), 196(2), 329-41
CODEN: EJBCAI; ISSN: 0014-2956
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Aspartate aminotransferase undergoes major shifts in the conformational equilibrium of the **protein matrix** during transamination. The present study defines the two conformational states of the enzyme by crystallog. anal., examines the conditions under which the enzyme crystallizes in each of these conformations, and correlates these conditions with the conformational behavior of the enzyme in solution, as monitored by a fluorescent reporter group. **Cocrystn.** of chicken mitochondrial aspartate aminotransferase with inhibitors and covalent coenzyme-substrate adducts yields three different crystal forms. Unliganded enzyme forms triclinic crystals of the open conformation, the structure of which has been solved (space group P1) [Ford, G. C., et al. (1980); Kirsch, J. F., et al. (1984)]. Complexes of the enzyme with dicarboxylate ligands form monoclinic or orthorhombic crystals of the closed conformation. The results of structure detns. of the latter two

crystal forms at 0.44 nm resolution are described here. In the closed conformation, the small domain has undergone a rigid-body rotation of 12-14° which closes the active-site pocket. Shifts in the conformational equilibrium of aspartate aminotransferase in solution, as induced by substrates, substrate analogs and specific dicarboxylic inhibitors, can be monitored by changes in the relative fluorescence yield of the enzyme labeled at Cys166 with monobromotrimethylammoniobimane. The pyridoxal and pyridoxamine forms of the labeled enzyme show the same fluorescence properties, whereas in the apoenzyme the fluorescence intensity is reduced by 30%. All active-site ligands, if added to the labeled pyridoxal enzyme at saturating concns., cause a decrease in the fluorescence intensity by 40-70% and a blue shift of maximally 5 nm. Comparison of the fluorescence properties of the enzyme in various functional states with the crystallog. data shows that both techniques probe the same conformational equilibrium The conformational change that closes the active site seems to be ligand-induced in the reaction of the pyridoxal form of the enzyme and syncatalytic in the reverse reaction with the pyridoxamine enzyme.

L20 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1981:98772 CAPLUS
DOCUMENT NUMBER: 94:98772
TITLE: Crystallization of yeast triose phosphate isomerase from polyethylene glycol. **Protein** crystal formation following phase separation
AUTHOR(S): Alber, Tom; Hartman, Fred C.; Johnson, Robert M.; Petsko, Gregory A.; Tsernoglou, Demetrius
CORPORATE SOURCE: Dep. Chem., Massachusetts Inst. Technol., Cambridge, MA, 02139, USA
SOURCE: Journal of Biological Chemistry (1981), 256(3), 1356-61
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A new crystal form of yeast triose phosphate isomerase (I) has been grown from solns. of the enzyme in polyethylene glycol (II) of average mol. weight 4000. The crystals are monoclinic, space group P21, with a = 61.3 Å, b = 98.4 Å, c = 49.7 Å, β = 90.9°. There is 1 dimeric mol./asym. unit. Data are observable to at least 1.3 Å resolution Crystallization can be achieved after the **protein** is induced to oil-out by II precipitation Small oil droplets of **protein** act as nucleation centers for the growth of large **single crystals**. Measurements of the **protein** and II content of the 2 phases of the yeast I system establish that the **protein** has gone entirely into the more dense phase. This phase also contains II. Consideration of the behavior of this 2-phase system suggests that II ppts. **proteins** at least in part by competing for water of hydration. Since the crystals can be stored in mother liquor which does not contain either sulfate or phosphate, substrate binding expts. can be carried out in the absence of competition by these anions. Addition of even low concns. of the transition state analog, 2-phosphoglycolate (III), to the native mother liquor causes the native enzyme crystals to dissolve. **Cocrystn.** of yeast I and III in the presence of II-4000 yields monoclinic crystals (space group P21, a = 74.2 Å, b = 82.9 Å, c = 37.6 Å, β = 102.0°) which diffract to better than 2.0 Å resolution Addition of the substrate, dihydroxyacetone phosphate, to the native mother liquor decreases the stability of the crystals in the x-ray beam, but diffraction is observed to at least 1.8 Å resolution Consequently, the yeast I system is suitable for a detailed mechanistic study of the reaction pathway.

L20 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1974:531798 CAPLUS
DOCUMENT NUMBER: 81:131798
TITLE: Change in the solubility of crystalline Fraction I **proteins** correlated with change in the composition of the small subunit
AUTHOR(S): Sakano, Katsuhiro; Kung, S. D.; Wildman, S. G.
CORPORATE SOURCE: Mol. Biol. Inst., Univ. California, Los Angeles, CA, USA
SOURCE: Plant and Cell Physiology (1974), 15(4), 611-17
CODEN: PCPHA5; ISSN: 0032-0781
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Fraction I **protein** crystals were obtained by a simple method from 4 addnl. species in addition to the 7 species of Nicotiana previously reported (Singh, S.; Wildman, S. G., 1973) and from Solanum melongena. Crystals were obtained neither from several other genera of the Solanaceal nor from N. debneyi, but 14C-labeled **protein** from the latter

cocrystd. with N. tabacum Fraction I **protein**. **Cocrystn** . did not occur with 14C-labeled **proteins** from species of Tagetes, Allium, Beta, Brassica and Hyocyamus, whose Fraction I **proteins** were evidently too different in their quaternarystructures to occupy the same crystal **lattice** with N. tabacum **protein**. Fraction I **proteins** from N. gossei and N. excelsior differed in solubility as a function of the NaCl concentration The 2 **proteins** were alike in the isoelec. point of the 3 primary peptides composing the large subunit, but differed in the isoelec. point of 1 out of 4 primary peptides of the small subunit; this difference was also consistent with a difference in tryptic peptide fingerprints. **Proteins** from N. tabacum and N. glauca differed both in the composition of their large and small subunits but did not differ in solubility However, by changing the composition of the small subunit without changing the large subunit, the solubility of each **protein** was changed. The change in small subunit composition was achieved by isolating **proteins** from the reciprocal F1 hybrids of N. tabacum + N. glauca where the maternal inheritance regulated the composition of the large subunit, whereas both maternal and paternal genes regulate the composition of the small subunit.

L20 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1972:484649 CAPLUS
DOCUMENT NUMBER: 77:84649
TITLE: Stereochemistry of actinomycin binding to DNA. I. Refinement and further structural details of the actinomycin-deoxyguanosine crystalline complex
AUTHOR(S): Jain, S. C.; Sobell, Henry M.
CORPORATE SOURCE: Dep. Chem., Univ. Rochester, Rochester, NY, USA
SOURCE: Journal of Molecular Biology (1972), 68(1), 1-20
CODEN: JMOBAK; ISSN: 0022-2836
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Actinomycin D (I) cocrystallizes with deoxyguanosine (II) to form a 1:2 stoichiometric complex. The crystals are orthorhombic, space group P212121, with cell parameters, a = 24.78, b = 29.47, and c = 13.60 Å. The structure contains 140 atoms in the asym. unit (1 I, 2 II, and 12 water mols.) and has been solved using a combination of Patterson and tangent refinement methods, and refined by full **matrix**-least squares to a residual of 9.4%. The 2 polypeptide chains of I are related by an approx. dyad axis lying roughly along a vector connecting the O-N bridging atoms in the phenoxazone ring. A strong H bond exists between neighboring cyclic pentapeptide chains connecting the N-H of 1 D-valine residue with the carbonyl O of the other D-valine residue (2.94, 2.96 Å). The conformations of the peptide linkages are as follows: L-threonine-D-valine, trans; D-valine-L-proline, cis; L-proline-sarcosine, cis; sarcosine-L-methylvaline, trans; L-threonine-carboxamide carbonyl O and C of chromophore, trans. The 1:2 stoichiometry of the complex is a direct consequence of the 2-fold sym. of I and reflects the 2 chemical equivalent binding sites available to II for complex formation. The 2 II mols. interact with each cyclic peptide residue and stack on alternate sides of the phenoxazone ring system. A strong H bond (2.82, 2.80 Å) connects the guanine 2-amino group with the carbonyl O of the L-threonine residue, while a weaker H bond connects the guanine N(3) ring N with the N-H group on this same L-threonine residue (3.15, 3.25 Å). Further details of the crystal structure are presented. This structure is an example of a **protein**-nucleic acid **cocrystn**. and the configuration observed in the crystalline complex explains in a natural way the stereochemistry of I binding to DNA.

L25 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:612528 CAPLUS
DOCUMENT NUMBER: 135:354312
TITLE: Incorporation of fluorescent molecules and **proteins** into calcium oxalate monohydrate **single crystals**
AUTHOR(S): Touryan, L. A.; Clark, R. H.; Gurney, R. W.; Stayton, P. S.; Kahr, B.; Vogel, V.
CORPORATE SOURCE: Department of Bioengineering, University of Washington, Seattle, WA, 98195, USA
SOURCE: Journal of Crystal Growth (2001), 233(1-2), 380-388
CODEN: JCRGAE; ISSN: 0022-0248
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A central question to understanding biomineralization is determining how biomols. are integrated within inorg. host **lattices**, thereby changing material properties yet retaining **single crystal structure** of the biomineral. We have addressed guest incorporation within single biomineral crystals by investigating face specificity, anisotropy and the role of charges in fluorescent calcium oxalate monohydrate (COM) crystals nucleated from solns. containing eosin Y, fluoresceins and rhodamines. Addnl., we have examined the specificity of incorporation of **Protein** G wild-type (G-wt) and its mutant (G-Δ6, in which four aspartic acids and two glutamic acids have been replaced by the corresponding asparagine or glutamine), where G-wt promotes and G-Δ6 inhibits COM crystal growth. We found that (1) the neg. charged fluorophores, as well as the fluorophore-labeled **proteins**, G-wt and G-Δ6, were successfully incorporated during growth into the same {110} growth sectors in preference to all others; (2) the pos. charged TRITC (tetra-Me rhodamine isothiocyanate) was not incorporated as free fluorophore, but it became incorporated if conjugated to G-wt and G-Δ6; (3) once the fluorophores are incorporated, the polarization measurements of adsorption and emission were similar irresp. whether taken from COM containing the free fluorophores, or the **protein** conjugates. The anisotropy was similar for rhodamines and fluoresceins.
REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:277190 CAPLUS
DOCUMENT NUMBER: 133:27835
TITLE: Oxygen binding by α(Fe2+)2β(Ni2+)2 hemoglobin crystals
AUTHOR(S): Bruno, Stefano; Bettati, Stefano; Manfredini, Michele; Mozzarelli, Andrea; Bolognesi, Martino; Deriu, Daniela; Rosano, Camillo; Tsuneshige, Antonio; Yonetani, Takashi; Henry, Eric R.
CORPORATE SOURCE: Institute of Biochemical Sciences, University of Parma, Parma, 43100, Italy
SOURCE: Protein Science (2000), 9(4), 683-692
CODEN: PRCIEI; ISSN: 0961-8368
PUBLISHER: Cambridge University Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Oxygen binding by Hb fixed in the T state either by **crystn.** or by encapsulation in silica gels is apparently noncooperative. However, cooperativity might be masked by different oxygen affinities of α and β subunits. Metal hybrid Hbs, where the noniron metal does not bind oxygen, provide the opportunity to determine the oxygen affinities of α and β hemes sep. Previous studies have characterized the oxygen binding by α(Ni2+)2β(Fe2+)2 crystals. Here, we have determined the three-dimensional (3D) structure and oxygen binding of α(Fe2+)2β(Ni2+)2 crystals grown from polyethylene glycol solns. Polarized absorption spectra were recorded at different oxygen pressures with light polarized parallel either to the b or c crystal axis by **single crystal** microspectrophotometry. The oxygen pressures at 50% saturation (p50s) are 95 ± 3 and 87 ± 4 Torr along the b and c crystal axes, resp., and the corresponding Hill coeffs. are 0.96 ± 0.06 and 0.90 ± 0.03. Anal. of the binding curves, taking into account the different projections of the α hemes along the optical directions, indicates that the oxygen affinity of α1 hemes is 1.3-fold lower than α2 hemes. Inspection of the 3D structure suggests that this inequivalence may arise from packing interactions of the Hb tetramer within the monoclinic crystal **lattice**. A similar inequivalence was found for the β subunits of

α(Ni2+)2β(Fe2+)2 crystals. The average oxygen affinity of the α subunits (p50 = 91 Torr) is about 1.2-fold higher than the β subunits (p50 = 110 Torr). In the absence of cooperativity, this heterogeneity yields an oxygen binding curve of Hb A with a Hill coefficient of 0.999. Since the binding curves of Hb A crystals exhibit a Hill coefficient very close to unity, these findings indicate that oxygen binding by T-state Hb is noncooperative, in keeping with the Monod, Wyman, and Changeux model.

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:751229 CAPLUS
DOCUMENT NUMBER: 132:32441
TITLE: Preparation and preliminary study of crystals of the recombinant calcium-regulated photoprotein obelin from the bioluminescent hydroid Obelia longissima
AUTHOR(S): Vysotski, Eugene S.; Liu, Zhi-Jie; Rose, John; Wang, B. C.; Lee, John
CORPORATE SOURCE: Photobiology Laboratory, Institute of Biophysics, Russian Academy of Sciences, Krasnoyarsk, 660036, Russia
SOURCE: Acta Crystallographica, Section D: Biological Crystallography (1999), D55(11), 1965-1966
CODEN: ABCRE6; ISSN: 0907-4449
PUBLISHER: Munksgaard International Publishers Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Crystals of recombinant obelin, the Ca2+-regulated photoprotein from the marine hydroid, O. longissima, were grown from Na citrate solns. The crystals grew as hexagonal light-yellow rods (0.1 + 0.1 + 1.0 mm) which diffracted to beyond 1.8 Å with synchrotron radiation of 1.0 Å wavelength. The crystals had a primitive hexagonal **lattice** with unit-cell parameters a = 81.55, c = 86.95 Å. The asym. unit contained 2 mols. This represented the successful preparation of **single crystals** of a photoprotein, obelin, which have promising diffraction properties.
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:224839 CAPLUS
DOCUMENT NUMBER: 128:293776
TITLE: Three-dimensional structure of a human Fab with high affinity for tetanus toxoid
AUTHOR(S): Faber, Catherine; Shan, Lin; Fan, Zhao-Chang; Guddat, Luke W.; Furebring, Christina; Ohlin, Mats; Borrebaeck, Carl A. K.; Edmundson, Allen B.
CORPORATE SOURCE: Oklahoma Medical Research Foundation, Oklahoma City, OK, 73104, USA
SOURCE: Immunotechnology (1998), 3(4), 253-270
CODEN: IOTEER; ISSN: 1380-2933
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The wide range of antibody specificity and affinity results from the differing shapes and chemical compns. of their binding sites. These shapes range from discrete grooves in antibodies elicited by linear oligomers of nucleotides and carbohydrates to shallow depressions or flat surfaces for accommodation of **proteins**, peptides, and large organic compds. The aim here was to determine the Fab structure of a high-affinity human antitoxin antibody; to explore structural features which enable the antibody to bind to intact tetanus toxoid, peptides derived from the sequence of the natural immunogen, and antigenic mimics identified by combinatorial chemical; to explain why this Fab shows a remarkable tendency to produce crystals consistently diffracting to d. spacings of 1.7-1.8; to use this information to engineer a strong tendency to crystallize into the design of other Fabs. The **protein** was crystallized in hanging or sitting drops by a microseeding technique in polyethylene glycol (PEG) 8000. Crystals were subjected to x-ray anal. and the 3-dimensional structure of the Fab was determined by the mol. replacement method. Interactive computer graphics were employed to fit models to electron d. maps, survey the structure in multiple views, and discover the crystal packing motif of the **protein**. Exceptionally large **single crystals** of this **protein** have been obtained, one measuring 5 + 3 + 2 mm (l + w + d). The latter was cut into 6 irregular pieces, each retaining the features of the original in diffracting to high resolution (1.8 Å) with little decay in the x-ray beam. In an individual

Fab, the active site is relatively flat and it seems likely that the **protein** antigen and derivative peptides are tightly held on the outer surface without penetration into the interior. There is no free space to accommodate even a dipeptide between VH and VL. One of the unique features of the B7-15A2 Fab is a large aliphatic ridge dominating the center of the active site. The CDR3 of the H chain contributes to this ridge, as well as to adjoining regions projected to be important for the docking of the antigen. Both the ease of **crystn.** and the favorable diffraction properties are mainly attributable to the tight packing of the **protein** mols. in the crystal **lattice**. The B7-15A2 active site provides a stable and well defined platform for high affinity docking of **proteins**, peptides, and their mimotopes. The advantages for future developments are suggested by the anal. of the crystal properties. It should be possible to incorporate the features promoting **crystn.**, close packing, and resistance to radiation damage into engineered human antibodies without altering the desired specificities and affinities of their active sites.

REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1994:264477 CAPLUS
DOCUMENT NUMBER: 120:264477
TITLE: Characterization, **crystallization** and preliminary X-ray crystallographic analysis of the complex between barley α-amylase and the bifunctional α-amylase/subtilisin inhibitor from barley seeds
AUTHOR(S): Vallee, Francois; Kadziola, Anders; Bourne, Yves; Abe, Junichi; Svensson, Birte; Haser, Richard
CORPORATE SOURCE: Lab. Cristallogr. Crist. Macromol. Biol., Univ. Aix-Marseille II, Marseille, 13916, Fr.
SOURCE: Journal of Molecular Biology (1994), 236(1), 368-71
CODEN: JMOBAK; ISSN: 0022-2836
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The complex between a member of the barley malt α-amylase isoenzyme 2 family (AMY2-2), and the endogenous bifunctional α-amylase/subtilisin inhibitor, BASI, was crystallized by the hanging drop vapor diffusion technique at a AMY2-2:BASI molar ratio of 1:1. The crystals were grown within 4 days from solns. containing polyethylene glycol and CaCl2. Anal. of **single crystals** by gel electrophoresis showed the presence of both **proteins** in the crystal **lattice**. The crystals belonged to orthorhombic space group P212121, with unit cell dimensions a = 74.5, b = 96.9, and c = 171.3 Å, and they diffracted to 2.0 Å resolution The preference of 2 mols. of the 1:1 complex in the asym. unit gave a solvent content of 45% by volume The 1:1 stoichiometry of the complex was confirmed by the mol. replacement method, using a search model the recently determined 3-dimensional structure of the barley α-amylase.

L25 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:181254 CAPLUS
DOCUMENT NUMBER: 114:181254
TITLE: **Crystallization** of mitochondrial creatine kinase. Growing of large **protein** crystals and electron microscopic investigation of microcrystals consisting of octamers
AUTHOR(S): Schnyder, Thomas; Winkler, Hanspeter; Gross, Heinz; Eppenberger, Hans M.; Wallimann, Theo
CORPORATE SOURCE: Inst. Cell Biol., Swiss Fed. Inst. Technol.-Hoenggerberg, Zurich, CH-8093, Switz.
SOURCE: Journal of Biological Chemistry (1991), 266(8), 5318-22
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Mitochondrial creatine kinase isolated from chicken cardiac muscle was crystallized by vapor diffusion techniques. Depending on the growth conditions, fine needles and platelets as well as large **single crystals** appeared after a few days. Large crystals were shown to diffract to at least 3.2-Å resolution and thus are suited for a detailed X-ray anal. in the future. The relatively high d. of **single crystals** measured by a linear organic solvent d. gradient indicates a tight packing of mitochondrial creatine kinase mols. within the crystals. Microcrystals, however, were subjected to electron optical examination either after prefixation with glutaraldehyde followed by conventional neg. staining or by freeze-fracturing crystals in mother liquid and heavy metal

replication with platinum/carbon. In both cases the crystals exhibited a square **lattice** with parameters of a = b = 139 Å and a = b = 132 Å in neg. stained and replicated crystals, resp. No other **lattice** parameters were found, suggesting that these microcrystals represent a quasi-cubic three-dimensional **lattice**, which is in accordance with the finding that the building blocks of the crystals are cube-like octamers. Digital image processing applied to electron micrographs of crystals clearly revealed the arrangement of mitochondrial creatine kinase octamers in the crystal **lattice** as well as the subdivision of the octamer into its subdomains at a resolution of 23 Å.

L25 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1975:134887 CAPLUS
DOCUMENT NUMBER: 82:134887
TITLE: **Crystallization** and preliminary x-ray investigation of soybean β-amylase
AUTHOR(S): Morita, Yuhei; Aibara, Shigeo; Yamashita, Honami; Yagi, Fumio; Suganuma, Toshihiko; Hiromi, Keitaro
CORPORATE SOURCE: Res. Inst. Food Sci., Kyoto Univ., Uji, Japan
SOURCE: Journal of Biochemistry (Tokyo, Japan) (1975), 77(2), 343-51
CODEN: JOBIAO; ISSN: 0021-924X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB β-Amylase was purified from defatted soybean meal by fractional precipitation with (NH4)2SO4(I), ion-exchange chromatog. on CM- and DEAE-Sephadex, and gel filtration chromatog. on Sephadex G 100. Two different components were crystallized from I solns., and the homogeneity of each preparation was confirmed by sedimentation and disc electrophoretic analyses. Both components formed large **single crystals** (trigonal crystal system) from 40-50% saturated I solution buffered at pH 5.4 on dialyzing concentrated **protein** solution Preliminary X-ray diffraction data gave a hexagonal **lattice** with unit cell dimensions a = 86.1 A and c = 144.4 A. The space group corresponds to P3121 or P3221, and 1 asymmetric unit contains 1 mol. of β-amylase, assuming a crystal d. of 1.25 g/ml and a mol. weight of 60,000 daltons. In this case, the crystal has a volume of 2.53 Å/atomic mass unit, and the percentage of **protein** in the crystal is .apprx.52.

L Number	Hits	Search Text	DB	Time stamp
1	31	"5075291"	USPAT; US-PGPUB	2004/03/24 08:45
2	51	chait.in.	USPAT; US-PGPUB	2004/03/24 08:49
3	0	rechtin.in	USPAT; US-PGPUB	2004/03/24 08:49
4	19	rechtin.in.	USPAT; US-PGPUB	2004/03/24 08:51
5	207930	protein polypeptide	USPAT; US-PGPUB	2004/03/24 08:51
6	152057	crystalliz$8 cocrystalliz$8	USPAT; US-PGPUB	2004/03/24 08:52
7	3314	(protein polypeptide) same (crystalliz$8 cocrystalliz$8)	USPAT; US-PGPUB	2004/03/24 08:52
8	424948	matrix lattice (single near4 crystal)	USPAT; US-PGPUB	2004/03/24 08:52
9	1897	((protein polypeptide) same (crystalliz$8 cocrystalliz$8)) and (matrix lattice (single near4 crystal))	USPAT; US-PGPUB	2004/03/24 08:52
10	380436	host guest inclusion entrap$4	USPAT; US-PGPUB	2004/03/24 08:53
11	1367	(((protein polypeptide) same (crystalliz$8 cocrystalliz$8)) and (matrix lattice (single near4 crystal))) and (host guest inclusion entrap$4)	USPAT; US-PGPUB	2004/03/24 08:53
12	387	((protein polypeptide) same (crystalliz$8 cocrystalliz$8)) same (matrix lattice (single near4 crystal))	USPAT; US-PGPUB	2004/03/24 08:54
13	250	(((protein polypeptide) same (crystalliz$8 cocrystalliz$8)) and (matrix lattice (single near4 crystal))) and (host guest inclusion entrap$4) and (((protein polypeptide) same (crystalliz$8 cocrystalliz$8)) same (matrix lattice (single near4 crystal)))	USPAT; US-PGPUB	2004/03/24 08:54